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Development of Physics-Based Numerical Models for Uncertainty Quantification of Selective Laser Melting Processes - 2015 Annual Progress Report

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1. GRANT OVERVIEW

<table>
<tr><td colspan="2" align="center">ESI CONTINUATION REVIEW PROPOSAL
NASA Grant NNX15AD81G

October 9, 2015

Development of Physics-Based Numerical Models for Uncertainty Quantification of Selective Laser Melting Processes

University of California, Davis</td></tr>
<tr><td>Principal Investigator</td><td>Jean-Pierre Delplanque</td></tr>
<tr><td>Research Collaborator</td><td>Kevin Wheeler
Ames Research Center</td></tr>
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2. RESEARCH OBJECTIVE

The primary goal of the proposed research is to characterize the influence of process parameter variability inherent to Selective Laser Melting (SLM) on components manufactured with the SLM technique for space flight systems and their performance. The current report covers the performance period from January 16 to April 16, 2015. Specific objectives are:

- To develop, verify, and validate robust physics-based numerical models for predictive SLM simulation using a DOE multi-physics, multi-scale massively parallel code called ALE3D for powder-scale SLM process simulations.
- To quantify the uncertainty in the prediction of material density and maximum tensile residual stress during laser melting and solidification of cubic coupons.

Increasingly demanding space missions require structures and equipment that perform better, are lighter, and more affordable than those produced using more traditional manufacturing methods. Additive manufacturing techniques, and SLM in particular, have a demonstrated capacity to manufacture such components. In fact, a recent report of the National Research Council[1] emphasizes the potential of additive manufacturing for the development of aerospace systems with increased performance. However, the adoption of these relatively new manufacturing techniques for the development of space systems will require the integration of computational techniques in the certification process of such components. The proposed project is a necessary step toward a scientifically-based numerical prediction of the SLM process which will enable the certification of components manufactured using SLM techniques for use in mission-critical roles.

[1] Committee on Space-Based Additive Manufacturing; Aeronautics and Space Engineering Board; National Materials and Manufacturing Board; Division on Engineering and Physical Sciences; National Research Council, 3D Printing in Space, The National Academies Press, 2014

3. MOST SIGNIFICANT TECHNICAL ACHIEVEMENT(S)

- Formulated points of collaboration with NASA Ames and LLNL regarding the development of a UQ strategy and the performance of detailed numerical simulations.
- Modified the direct metal deposition facility for single track laser melting experiments
- Successfully designed and performed the first two sets of single-track laser melting experiments.
- To ascertain the influence of powder morphology, characterized and quantified the differences in morphology and size distribution between 316L stainless steel powders produced by water atomization and gas atomization.
- Characterized density of single track samples using image analysis.
- Proposed Volumetric Energy Density as a possible characteristic process parameter.
- Powder flowability was experimentally investigated with deposition on an inclined stage. Macroscopic differences were observed between the powders obtained by water atomization and gas atomization.
- Third set of single-track experiments has been designed and baseplates are being prepared.
- Explored forward uncertainty propagation techniques with a simple test surrogate model using DAKOTA.
- Explored Bayesian Inference techniques for uncertainty quantification with a simple test surrogate model and manufactured data.
- Performed preliminary simulation using ALE3D.

4. ACTIVITIES AND ACCOMPLISHMENTS

Activities during this reporting period have focused on establishing the foundation required to progress towards Year 1 milestones as briefly discussed below

- **Activities Relevant to Milestone 1: "Develop a UQ strategy based on a simple thermal model"**

  Preliminary work with one of the possible UQ tools (DAKOTA) has been initiated. Plans are being made for a graduate student to spend part of the summer at Ames to interact with NASA collaborators on the topic of uncertainty quantification.

  A simple 1D thermal model was used as a test case to investigate and compare various forward UQ techniques. In addition to applying these techniques manually (in Matlab), the UQ tool DAKOTA was utilized to perform the same analyses.

  The exploration of Bayesian inference (Figure 1) was initiated, working closely with NASA collaborators. A few inverse UQ example problems were successfully implemented, including an example utilizing multiple ALE3D runs, showcasing a framework for future UQ strategies.

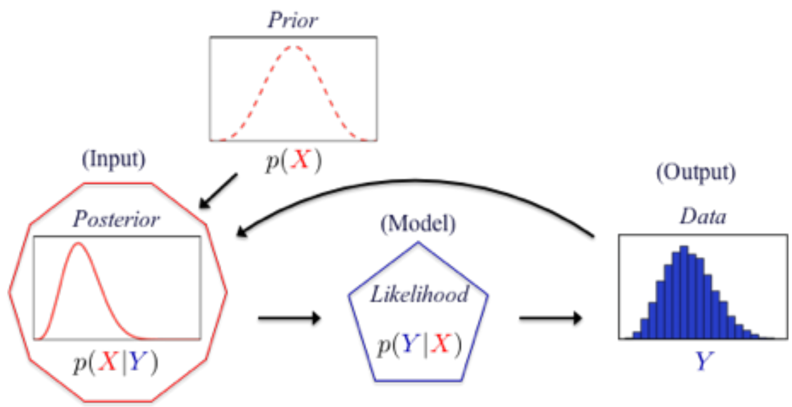

Figure 1: Bayesian Inference Process

- **Activities Relevant to Milestone 2: "Perform preliminary runs with ALE3D"**

A graduate student was trained at LLNL over the summer to run ALE3D. Preliminary runs focused on a reduced version of the cases reported by Khairallah and Anderson[2]. A 0.1mm x 0.1mm x 0.2mm stainless steel power bed was considered with a stationary Laser applied at the center of the domain for 20 μs (Figure 2).

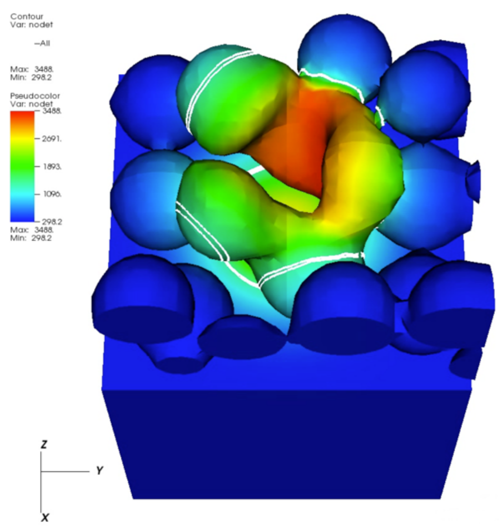

Figure 2: Sample, scaled-down, SLM simulation. Stationary 300W laser applied for 20 μs to a small single layer powder bed. The white lines represent the solidus and liquidus isotherms.

A directory of existing ALE3D runs relevant to the SLM process is being constructed.

A 2D inverse UQ problem for formulated and solved using ALE3D (Figure 3). In addition to providing troubleshooting experience with the code for the researcher, this example served to develop a scheme for running multiple iterations of ALE3D in a UQ context.

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[2] Khairallah, S.A. and Anderson, A. , "Mesoscopic simulation model of selective laser melting of stainless steel powder," *Journal of Materials Processing Technology* 214 2627--2636 (2014)

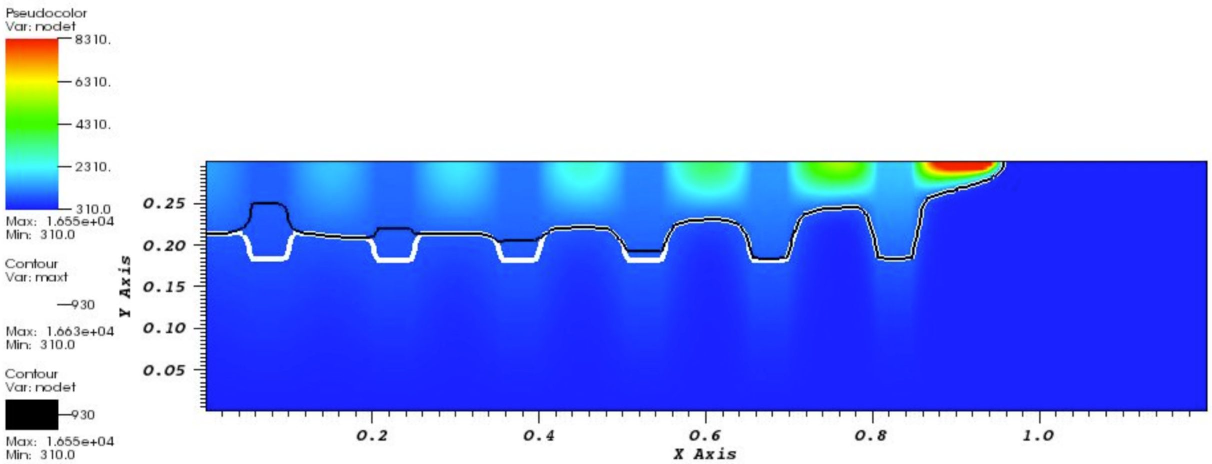


Figure 3: ALE3D simulation of the thermal conductivity step function UQ problem The flooded contours denote temperature; the black line is the instantaneous position of the solid/liquid front, and the white line is the locus of largest melt depth [LLNL-PRES-677661]

An End-User agreement request was submitted by UC Davis to enable continued access for the rest of the project.

- **Activities Relevant to Milestone 3: "Modify direct metal deposition facility for laser melting experiments"**

  The modifications needed to allow single-track laser melting experiments and multiple-pass experiments have been identified. The lens needed for the former (focal length 300 mm) has been procured and installed. The system has been calibrated for the new configuration. Preliminary concepts for the successive deposition of powders layers are being formulated.

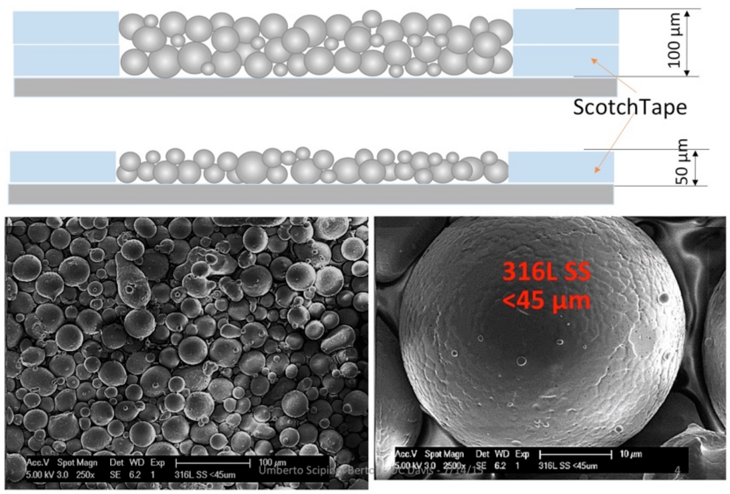
  Laser upgrade from the current Nd-YAG laser to a state-of-the-art fiber laser is currently ongoing.

- **Activities Relevant to Milestone 4: "Initiate single-track laser melting experiments."**

  Graduate student has been trained on using the direct metal deposition system. Literature review has been initiated.

  Performed first set of single-track deposition experiments – Powder layer thickness was controlled either with maximum powder size or with a layer of adhesive tape (Fig. 4). The latter achieved full melting of the track (Fig. 5) when the right combination of deposition parameters was chosen (laser power/working distance/powder particle size).

  Performed characterization of 316L ordered powders – Two batches of 316L stainless steel powders are available: one gas-atomized and the other water-atomized. We performed a full characterization of the powders in terms of particle shape, particle size, particle size distribution, packing density of the powder and its chemical composition.



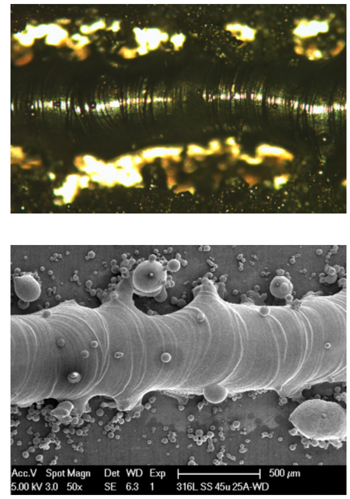


Figure 4: Controlling powder layer thickness via additive layers of tape.

Figure 5: Single track morphology.

Powder packing characterization and modeling is investigated numerically first to provide the insight needed to build simulations that are representative of the powders and configurations used experimentally.

Second set of single-track experiments was performed on a deep powder bed (~10 mm) for easy single-tracks extraction. Different values of Energy Density were employed and their correlation with the samples' final dimensions were assessed. Severe balling was observed when water atomized powder was used.

Density of single tracks was measured with image analysis after polishing. All samples showed near-full density (>99.5%)

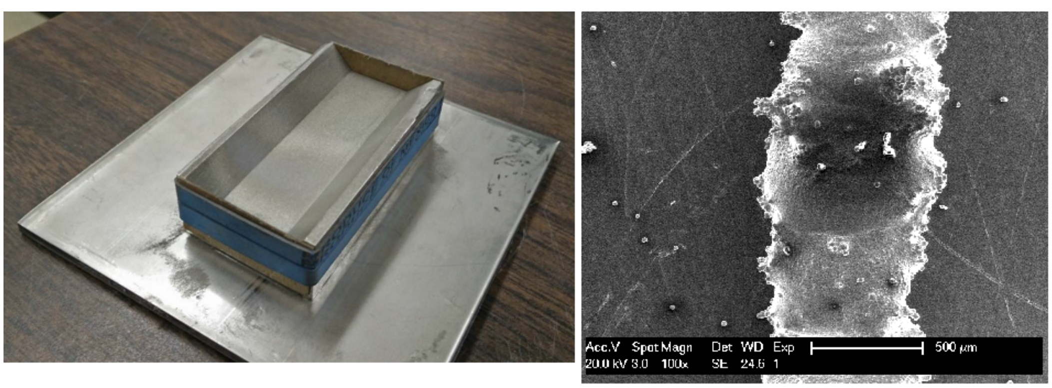


Figure 6: Support for powder bed (left) and single track after deposition (right)

Preliminary flowability tests on powders were performed on an inclined platform. Water atomized powder seems to flow better than the gas atomized which instead clumps more easily. Heating both the substrate and the gas atomized powder helped increasing the flowability of the latter.

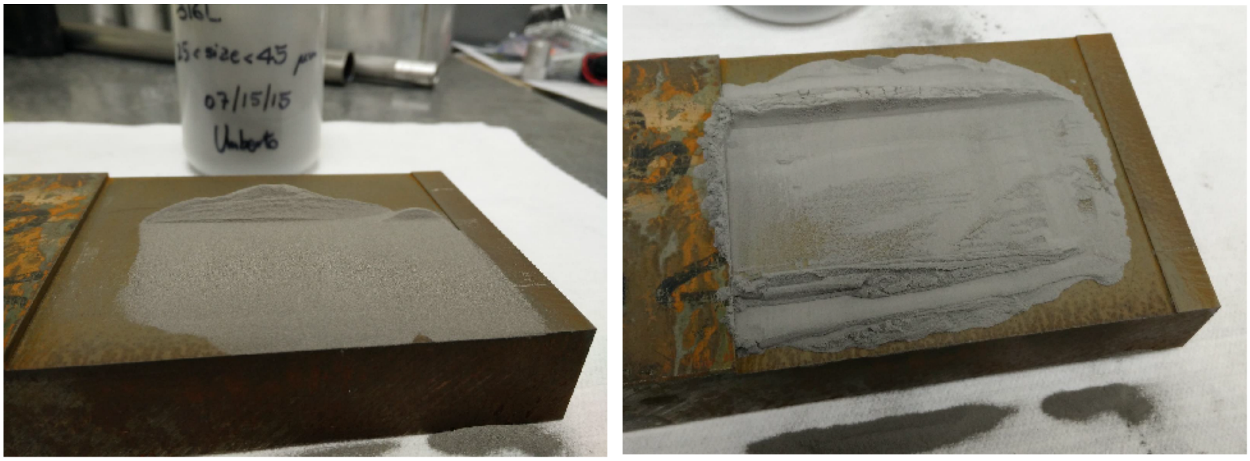


Figure 7: Water atomized powder (left) is easily spread to form a neat and even layer while gas atomized powder (right) tends to clump and has generally poorer flowability.

5. PLANNED ACTIVITIES

The activities planned for the remaining grant award period include (organized according to Year 1 milestones):

- **Planned Activities Relevant to Milestone 1: "Develop a UQ strategy based on a simple thermal model"**
  - Continue to research inverse UQ problems, using more advanced techniques. These techniques will enable the identification of process (input) parameters that primarily contribute to the variability of the quantities of interest.
  - Evaluate the use of DAKOTA Bayesian UQ capabilities for the SLM analysis.
  - Develop simple but more relevant test problems to test various UQ strategies

- **Planned Activities Relevant to Milestone 2: "Perform preliminary runs with ALE3D"**
  - Expand on existing preliminary ALE3D run to include Inconel cases.
  - Perform basic test case simulations of the single-track geometry.

- **Planned Activities Relevant to Milestone 3: "Modify direct metal deposition facility for laser melting experiments"**
  - The modification of the facility is currently ongoing.

- **Planned Activities Relevant to Milestone 4: "Initiate single-track laser melting experiments."**
  - Continue single-track experiments with different powder-bed approaches (e.g. inclined stage to assess variation of layer thickness).
  - High-speed imaging of the dynamics of powder particles (or larger 316l SS balls) in the melt pool during laser powder bed melting;
  - Non-contact thermal imaging measurement will be used to investigate the thermal behavior within and near a molten pool;
  - Physical simulation of powder particles melting and merging in melt pool with larger 316l SS balls, using an unfocused laser beam for slowly heat up. The data thus acquire will be used for partial validation of SLM relevant numerical simulations.

6. NASA COLLABORATION

From the beginning of the summer until the end of July, a graduate student spent two days a week at Ames Research Center. Through interactions with NASA collaborators, the student gained understanding of Bayesian inference and inverse UQ, and was mentored through several example problems. In addition, the student was exposed to a variety of concepts that will be useful in future UQ efforts (such as Gaussian process regression and maximum entropy probability distributions).

After the student's time at Ames, periodic updates with NASA collaborators were conducted over email, phone, or GoToMeeting.

A kick-off meeting (at UC Davis on 20 March 2015) and three technical update meetings (14 May 2015 at UC Davis and 28 July 2015 and 20 September 2015, both at LLNL) were organized with participation of the UC Davis team, the LLNL collaborators and the NASA collaborators. The meetings at LLNL included sessions with LLN UQ and real-time diagnostics researchers as well as a visit of the real-time diagnostics facilities pertaining to additive manufacturing.

7. ANNUAL TECHNICAL SEMINARS

Completed / Planned Annual Technical Seminars			
Award Year	***Date***	***NASA Center***	***Seminar Topic and Optional Comments***
1	23 SEP 2015	Ames RC	Research effort recently initiated at UC Davis in collaboration with LLNL and NASA Ames under the sponsorship of an Early Stage Innovations grant from NASA's Space Technology Research Grants Program to characterize the influence of process parameter variability inherent to SLM on components manufactured with that technique for space flight systems.
2			
3			

8. NEW TECHNOLOGY, REPORTABLE ITEMS, INVENTIONS, AND PATENTS

None at this time.

9. POSTDOCTORAL RESEARCHER(S) / STUDENT(S)

Assistance Type	**Number**	**Roles / Comments**
Postdoctoral	1	Supervision and contribution to the experimental effort. Partially funded by the ESI grant.

Graduate	2	Both directly funded by the ESI grant.
Undergraduate	1	Contribution to the experimental effort. University-funded.
Other	1	Participation in overall project supervision. University-funded.